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TITLE FINAL STATE EFFECTS IN NEUTRON SCATTERING EXPERIMENTS ON MOMENTUM DISTRIBUTIONS IN QUANTUM FLUIDS

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Final State Effects in Neutron Scattering Experiments on Momentum Distributions in Quantum Fluids

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Using a "hard core perturbation theory," the final state corrections to the impulse approximation are derived for high Q neutron scattering experiments to determine momentum distributions in quantum fluids. The final state broadening depends on the radial distribution function, g(r), and the He-He phase shifts. It has a zero second moment and no Lorentzian wings, satisfying the kinetic energy sum rule. Explicit results are presented for superfluid ^{4}He.

1. INTRODUCTION:

Since the original suggestion by Hohenberg & Platzman [1], there have been many experiments [2] to determine the momentum distributions in quantum solids and fluids by scattering neutrons at Q high enough to invoke the impulse approximation (IA). Most theories of the final state corrections to the IA have predicted a quasi-Lorentzian lineshape [3]. However, Gersch, et al. [4] argued that the real space correlations, expressed through g(r), result in a non-Lorentzian final state broadening. A simple quasiclassical theory for this effect was developed by Silver & Reiter [5].

In this paper, I outline the first perturbative derivation of the final state effects in deep inelastic neutron scattering experiments on quantum fluids. The vertex terms introduce g(r). I present numerical results for superfluid ^{4}He.

2. HARD CORE PERTURBATION THEORY:

First, I approximate the Hamiltonian at high Q. The long range part of the potential and the low momentum part of the kinetic energy govern the ground state properties such as g(r) and n(p). The short range part of the potential and the high momentum part of the kinetic energy dominate final state effects. I treat the former statically, with g(r) given by experiment or by other theory, and I carry out a perturbation expansion for the dynamics using the latter part of the Hamiltonian.

Second, a perturbation theory for hard core potentials (termed "HCPT") can be developed by analogy with the perturbative derivation of Boltzmann equation expressions for the electrical resistivity starting from the Kubo formula. The "diagonal projection operator method" of Argyres & Sigel [6] resums the terms in the Liouville perturbative expansion of the Kubo formula which are singular as $\omega \to i\varepsilon$ (i.e. from intermediate terms in the density matrix of form $a_k^{\dagger}a_k$). The perturbative expansion of $S(Q,\omega)$ is formally analogous, with the singular terms occurring as $\hbar\omega \to \hbar^2Q^2/2m + i\varepsilon$. To resum these singular terms (of form $a_{k+Q}^{\dagger}a_k$), I again perform a Liouville perturbative expansion of $S(Q,\omega)$, but with an off-diagonal density projection operator defined in terms of ground state expectation values. $S(Q,\omega)$ can then be written as a Dyson equation for a two particle propagator with the Liouville T-operator generating the irreducible part.

Assuming two-body collisions dominate the final state effects, the third step is to replace the many-body Liouville T operator by an unrenormalized two body T-operator. In the resultant theory, I evaluate expectation values in the ground state of products of two creation and two annihilation operators in terms of the g(r) and the momentum distributions in agreement with the sum rules. The self energy terms in the Dyson equation alone would predict quasi-Lorentzian lineshapes. However, the self energy terms are exactly canceled by a part of the vertex terms, which is related to a Ward identity.

The fourth step is to evaluate the high Q limit of the two body T-matrix using semiclassical methods [7]. This includes taking the T-matrix on-energy-shell, JWKB phase shifts, the Poisson summation formula, and the large L/small angle representation of the Legendre polynomials in terms of Bessel functions. The resulting Dyson equation may be solved analytically.

Details of these calculations will be given elsewhere.

3. RESULTS:

In the high Q limit of the HCPT, I find that $Q\,S(Q,\omega)$ is a convolution

$$Q\,S(Q,\omega) \equiv F(Y) = \int_{-\infty}^{\infty} dY'\, R_{HCPT}(Y-Y')\, F_{IA}(Y') \qquad (1)$$

where the scaling variable is $Y \equiv (\omega-\hbar Q^2/2m)m/\hbar Q$, and $F_{IA}(Y)$ is the impulse approximation result for $Q\,S(Q,\omega)$. The final state resolution function, $R_{HCPT}(Y)$, is given by

$$R_{HCPT}(Y) = \frac{1}{\pi}\int_0^{\infty} dX\, \cos\left(YX + \int_0^X dX'\, \mathrm{Re}\,\Gamma(X')\right) \cdot \exp\left(\int_0^X dX'\, \mathrm{Im}\,\Gamma(X')\right) \qquad (2)$$

$$\Gamma(X) = 2\pi\rho \int_0^{\infty} B\, dB\, f(B)\, g\left(\sqrt{X^2 + B^2}\right) \qquad (3)$$

and

$$f(B) = e^{2i\delta(B)} - 1 + \sum_{M\neq 0} e^{2i\delta(B)+iM\pi QB/2} \qquad (4)$$

Here, $\delta(B)$ is the JWKB phase shift for impact parameter B and ρ is the density. $\Gamma(\infty)$ is proportional to the He-He T-matrix. Note that this theory satisfies the kinetic energy sum rule even for hard sphere potentials.

Figure 1 compares [8] the final state broadening of HCPT to a Lorentzian (LZ) obtained by taking $g(r) \to 1$ in Eq. 3. R_{HCPT} has a zero second moment and no Lorentzian wings.

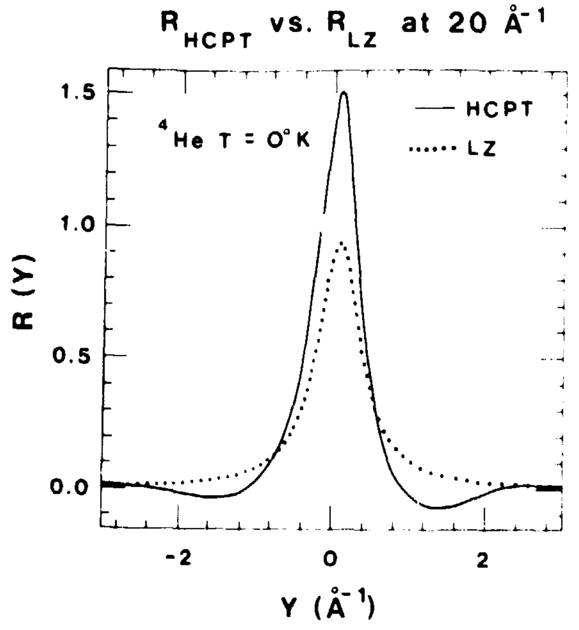

Fig. 1 Final state broadening function, R(Y), at $Q = 20\ Å^{-1}$ for hard core perturbation theory (HCPT) and Lorentzian broadening (LZ) vs. $Y \equiv (\omega - \hbar Q^2/2m)m/\hbar Q$.

Figure 2 shows calculations of Q S(Q,ω) using a theoretical momentum distribution of ^4He [9] at T = 0 °K which has an 11.9% Bose condensate fraction. For HCPT, the linewidth of the non-condensed atoms is comparable to the IA, but the Bose condensate peak is not clearly resolved. Because the He-He potential is steeply repulsive, a distinct condensate peak is not obtained even for Q's up to 100's $Å^{-1}$. The LZ lineshape is much wider than HCPT and IA. In addition, there are much smaller hard sphere glory oscillations of Q S(Q,ω) in HCPT than in LZ.

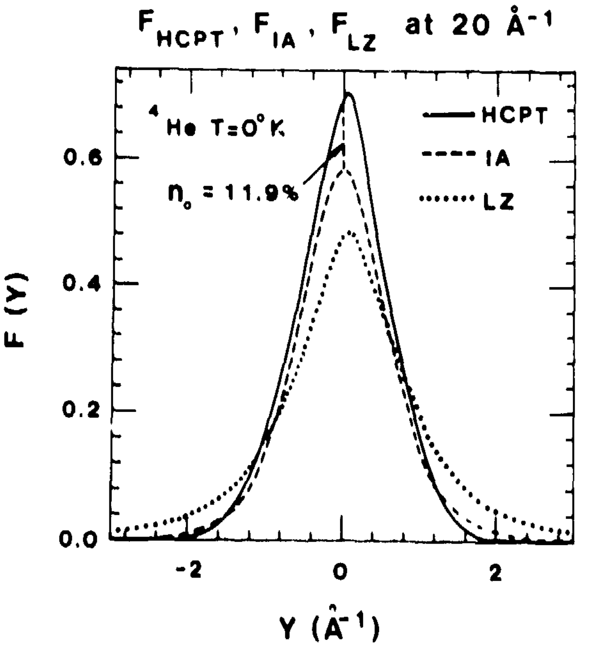

Fig. 2. $Q\,S(Q,\omega) \equiv F(Y)$ where $Y \equiv (\omega - \hbar Q^2/2m)m/\hbar Q$ for hard core perturbation theory (HCPT), impulse approximation (IA) and Lorentzian broadening (LZ) at $Q = 20\ Å^{-1}$.

4. CONCLUSION:

The hard core perturbation theory of deep inelastic neutron scattering experiments qualitatively confirms the earlier many-body cumulant theory of Gersch, et al. [4] and the quasiclassical theory of Silver & Reiter [5]. The quantitative predictions and the structure of the theory are new. I have shown how vertex corrections give rise to a non-Lorentzian, zero second moment lineshape for final state effects. The good news for experimentalists is that, at high enough Q, the final state broadening of the impulse approximation takes the form of a convolution and is smaller than the Lorentzian broadening theories would predict. The bad news is that neither the Bose condensate peak in ^4He nor the Fermi surface discontinuity in ^3He will be clearly resolved in S(Q,ω) in any feasible deep inelastic neutron scattering experiment. However, provided the final state theory is known and instrumental corrections understood, a deconvolution procedure (such as maximum entropy) might be attempted to extract the singular structures and other properties of momentum distributions. There must now be a detailed effort to reanalyze momentum distribution experiments on quantum fluids and solids. At lower Q, the assumptions underlying Eqs. 1-4 (such as on-energy-shell T-matrix) break down and the relation of n(p) to S(Q,ω) will be more complex. An extension of the HCPT should enable calculations at lower Q in the future.

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REFERENCES

1) P. C. Hohenberg, P. M. Platzman, Phys. Rev. 152, 198 (1966).
2) See, e.g. E. C. Svennson, Proceedings of the 1984 Workshop on High Energy Excitations in Condensed Matter, LA-10227, p. 456.
3) For references and discussion of other theories of final state effects, see R. N. Silver, G. Reiter, Phys. Rev. B1, 35, 3647 (1987).
4) H. A. Gersch, L. J. Rodriguez, Phys. Rev. A 8, 905 (1973); L. J. Rodriguez, H. A. Gersch, H. A. Mook, ibid., 9, 2085 (1974).
5) Ref. 3, ibid.
6) P. N. Argyres, J. L. Sigel, Phys. Rev. Letters 31, 1397 (1973); Phys. Rev. B 9, 3197 (1974).
7) See, e.g., M. V. Berry, K. E. Mount, Reports on Progress in Physics, 35, 315 (1972).
8) I use the He-He potential of R. Feltgen, H. Kirst, K. A. Kohler, H. Pauly, F. Torello, J. Chem. Phys. 76 (5), 2360 (1982) and the g(r) from E. C. Svennson, V. F. Sears, A. D. Woods, P. Martel, Phys. Rev. B 21, 3638 (1980).
9) P. M. Lam, J. W. Clark, M. L. Ristig, Phys. Rev. B 16, 222 (1977).